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Supporting Information

Five Novel Zn(II)/Cd(II) Coordination Polymers Based on Bis(pyrazinyl)-trizole and Varied Polycarboxylates: Syntheses, Topologies and Photoluminescences

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1. PXRD patterns of complexes **1-5**.

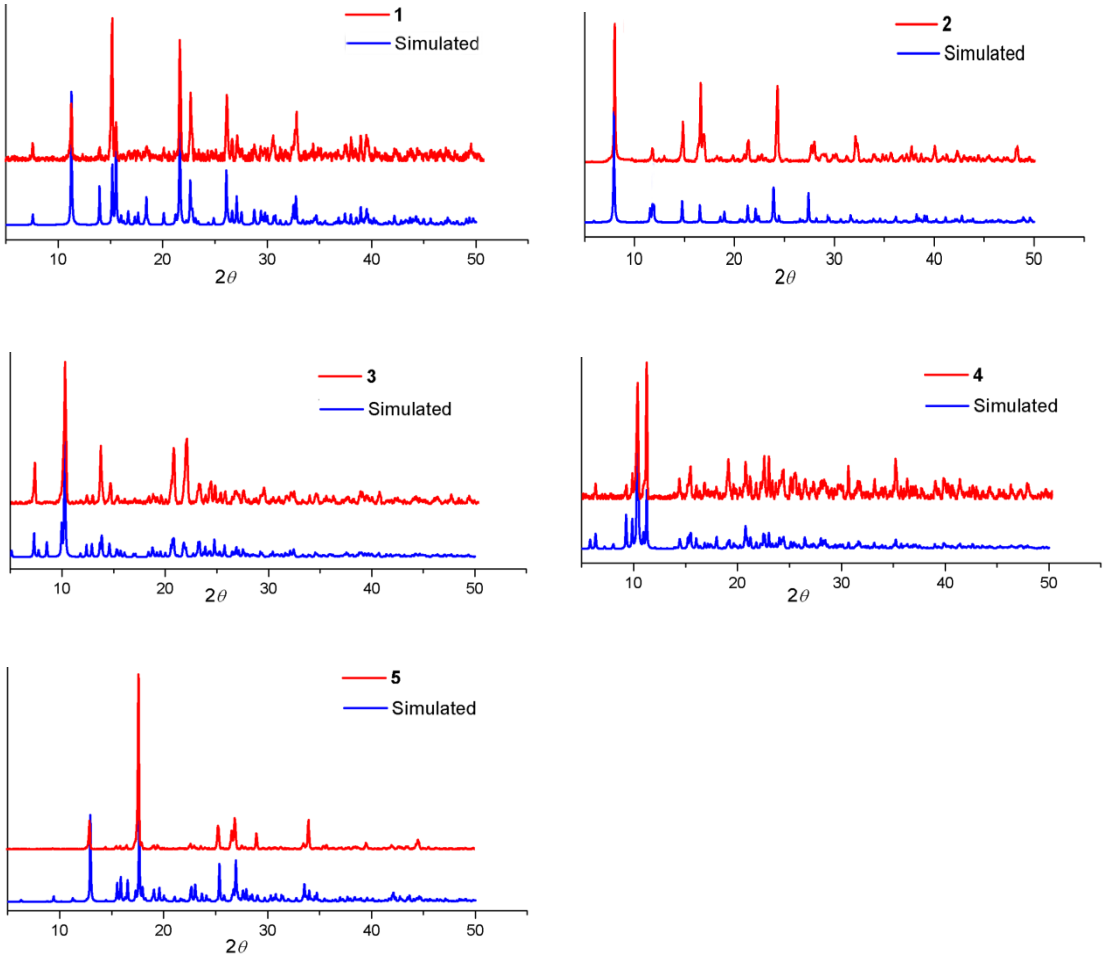


Figure S1. XRPD experimental and calculated patterns for complexes.

2. TGA curves for complexes **1-5**.

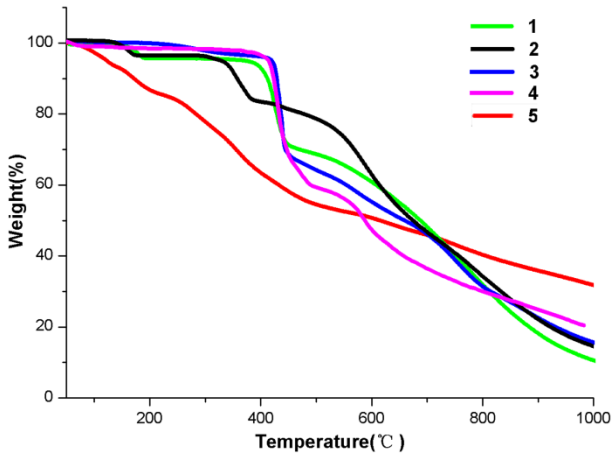


Figure S2. TGA curves for complexes **1-5**.

3. Solid-state emission spectra of the free ligands at 298K.

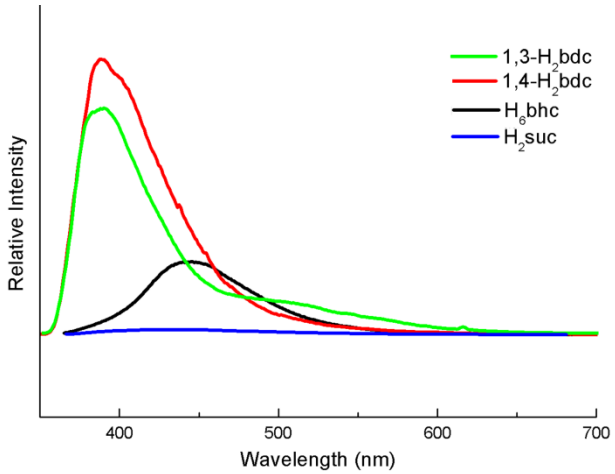
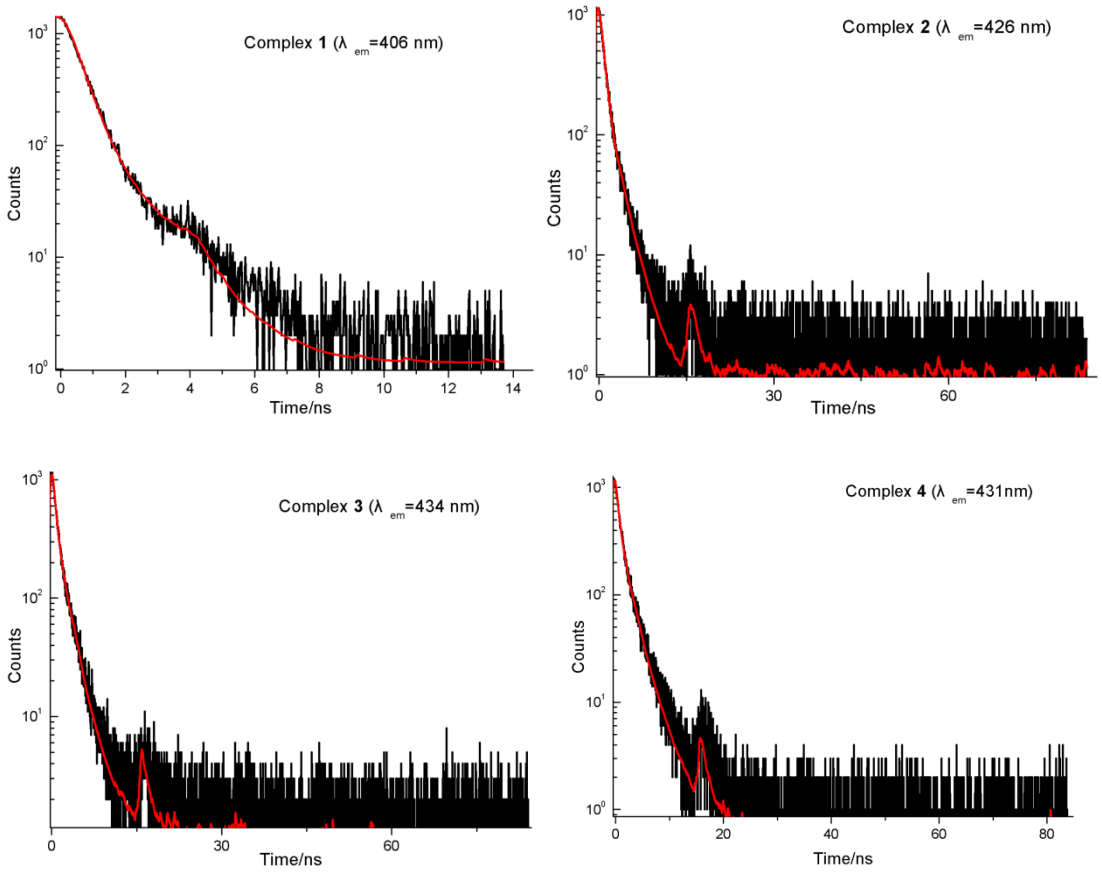


Figure S3. Solid state emission spectra of free polycarboxylates ligands.

4. Photoluminescence lifetimes of complexes **1**-**5**.



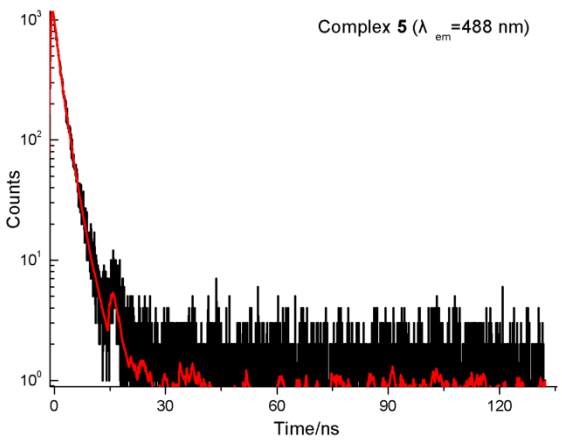


Figure S4. Luminescence decay curves for complexes **1-5**.

5. IR spectra of complexes **1-5**.

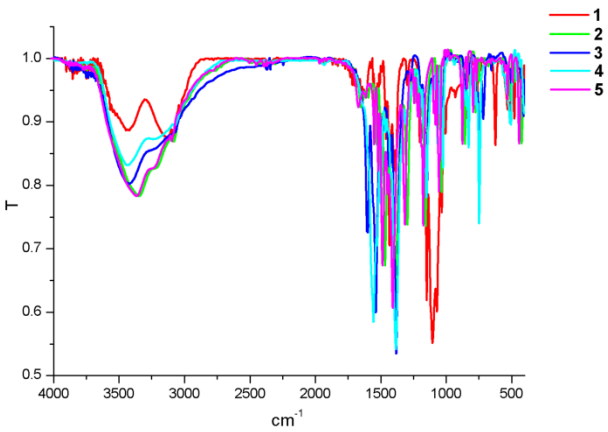


Figure S5. IR spectra of complexes **1-5**.

6. Selected bond lengths (Å) and angles (°) for complexes **1-5**.

Table S1. Selected Bond Lengths (Å) and Angles (°) for Complexes.

Complex **1**			
Cd1—O1	2.245 (4)	Cd1—N1^{ii}	2.396 (4)
Cd1—N5^{i}	2.264 (4)	Cd1—N2	2.432 (4)
Cd1—N3	2.303 (4)	Cd1—N6^{i}	2.493 (4)
O1—Cd1—N5^{i}	94.97 (15)	N3—Cd1—N2	74.80 (14)
O1—Cd1—N3	105.19 (15)	N1^{ii}—Cd1—N2	88.40 (15)
N5^{i}—Cd1—N3	155.89 (14)	O1—Cd1—N6^{i}	86.91 (16)
O1—Cd1—N1^{ii}	89.00 (17)	N5^{i}—Cd1—N6^{i}	69.01 (14)
N5^{i}—Cd1—N1^{ii}	98.32 (15)	N3—Cd1—N6^{i}	98.57 (14)
N3—Cd1—N1^{ii}	95.16 (14)	N1^{ii}—Cd1—N6^{i}	166.26 (15)
O1—Cd1—N2	177.39 (15)	N2—Cd1—N6^{i}	95.67 (15)
N5^{i}—Cd1—N2	85.65 (15)		

Symmetry codes: (i) x, 3/2-y, 1/2+z; (ii) 2-x, 1/2+y, 1/2-z; (iii) 2-x, -1/2+y, 1/2-z; (iv) x, 3/2-y, -1/2+z.

Complex **2**			
Cd1—O1	2.242 (5)	Cd3—N4	2.405 (9)
Cd1—O4^{iii}	2.265 (5)	Cd3—O12	2.44 (2)
Cd1—O5	2.354 (7)	Cd4—N8^{ii}	2.303 (6)
Cd1—N5	2.399 (7)	Cd4—O9	2.325 (8)
Cd1—O6	2.412 (7)	Cd4—N9	2.336 (6)
Cd1—N11^{iii}	2.417 (7)	Cd4—O8	2.354 (8)
Cd2—O2	2.305 (6)	Cd4—O7	2.551 (8)
Cd2—N14^{i}	2.339 (7)	Cd4—O10	2.569 (7)
Cd2—N1	2.344 (7)	Cd4—N10	2.583 (7)
Cd2—O3^{i}	2.403 (5)	Cd5—O10	2.178 (9)
Cd2—O4^{i}	2.468 (5)	Cd5—O10^{ii}	2.178 (9)
Cd2—O1	2.607 (5)	Cd5—N12	2.392 (10)
Cd3—O7^{ii}	2.192 (10)	Cd5—N12^{ii}	2.392 (10)
Cd3—O7	2.192 (10)	Cd5—O11	2.431 (18)
Cd3—N4^{ii}	2.405 (9)		
O1—Cd1—O4^{iii}	113.3 (2)	N4—Cd3—O12^{ii}	97.2 (6)
O1—Cd1—O5	141.1 (3)	O12—Cd3—O12^{ii}	24.6 (8)
O4^{iii}—Cd1—O5	100.9 (2)	N8^{ii}—Cd4—O9	109.2 (3)
O1—Cd1—N5	86.9 (3)	N8^{ii}—Cd4—N9	89.5 (2)
O4^{iii}—Cd1—N5	88.5 (2)	O9—Cd4—N9	126.9 (3)
O5—Cd1—N5	112.7 (3)	N8^{ii}—Cd4—O8	125.2 (3)
O1—Cd1—O6	101.8 (2)	O9—Cd4—O8	97.9 (4)
O4^{iii}—Cd1—O6	141.3 (3)	N9—Cd4—O8	111.0 (3)
O5—Cd1—O6	54.6 (2)	N8^{ii}—Cd4—O7	82.0 (3)
N5—Cd1—O6	77.4 (3)	O9—Cd4—O7	148.0 (3)
O1—Cd1—N11^{iii}	85.9 (3)	N9—Cd4—O7	81.7 (3)
O4^{iii}—Cd1—N11^{iii}	87.1 (2)	O8—Cd4—O7	53.8 (4)
O5—Cd1—N11^{iii}	77.7 (3)	N8^{ii}—Cd4—O10	80.4 (3)
N5—Cd1—N11^{iii}	169.3 (3)	O9—Cd4—O10	53.8 (3)
O6—Cd1—N11^{iii}	111.9 (3)	N9—Cd4—O10	83.1 (3)
N1—Cd2—O3^{i}	113.2 (2)	O8—Cd4—O10	149.3 (4)
O2—Cd2—O4^{i}	148.65 (18)	O7—Cd4—O10	156.8 (3)
N14^{i}—Cd2—O4^{i}	86.9 (3)	N8^{ii}—Cd4—N10	155.7 (2)
N1—Cd2—O4^{i}	82.1 (2)	O9—Cd4—N10	77.9 (3)
O3^{i}—Cd2—O4^{i}	52.44 (16)	N9—Cd4—N10	68.8 (2)
O2—Cd2—O1	52.18 (17)	O8—Cd4—N10	74.8 (3)
N14^{i}—Cd2—O1	82.1 (3)	O7—Cd4—N10	104.4 (3)
N1—Cd2—O1	80.5 (2)	O10—Cd4—N10	86.2 (3)
O3^{i}—Cd2—O1	146.71 (16)	O10—Cd5—O10^{ii}	111.3 (3)
O4^{i}—Cd2—O1	159.16 (16)	O10—Cd5—N12	85.0 (3)
O7^{ii}—Cd3—O7	113.7 (4)	O10^{ii}—Cd5—N12	89.7 (3)
O7^{ii}—Cd3—N4^{ii}	87.3 (4)	O10—Cd5—N12^{ii}	89.7 (3)

O7—Cd3—N4^{ii}	85.9 (4)	O10^{ii}—Cd5—N12^{ii}	85.0 (3)
O7^{ii}—Cd3—N4	85.9 (4)	N12—Cd5—N12^{ii}	170.6 (4)
O7—Cd3—N4	87.3 (4)	O10—Cd5—O11^{ii}	108.3 (6)
N4^{ii}—Cd3—N4	167.6 (4)	O10^{ii}—Cd5—O11^{ii}	140.3 (6)
O7^{ii}—Cd3—O12	110.9 (4)	N12—Cd5—O11^{ii}	94.3 (6)
O7—Cd3—O12	135.4 (5)	N12^{ii}—Cd5—O11^{ii}	94.7 (6)
N4^{ii}—Cd3—O12	97.2 (6)	O10—Cd5—O11	140.3 (6)
N4—Cd3—O12	94.9 (6)	O10^{ii}—Cd5—O11	108.3 (6)
O7^{ii}—Cd3—O12^{ii}	135.4 (5)	N12—Cd5—O11	94.7 (6)
O7—Cd3—O12^{ii}	110.9 (4)	N12^{ii}—Cd5—O11	94.3 (6)
N4^{ii}—Cd3—O12^{ii}	94.9 (6)	O11^{ii}—Cd5—O11	32.1 (12)
Symmetry codes: (i) 1/2+x, 1/2-y, -z; (ii) x, -y, -z; (iii) 1/2-x, 1/2-y, -1/2+z.			

Complex **3**			
Cd1—O4^{i}	2.184 (3)	Cd3—O9^{ii}	2.216 (4)
Cd1—N18^{i}	2.274 (4)	Cd3—N12	2.286 (4)
Cd1—O10^{v}	2.298 (4)	Cd3—N17	2.316 (4)
Cd1—N3	2.313 (4)	Cd3—O1	2.338 (3)
Cd1—N20^{i}	2.469 (4)	Cd3—N15	2.516 (4)
Cd1—N1	2.493 (4)	Cd3—N14	2.588 (4)
Cd2—N11	2.208 (4)	Cd4—O6	2.199 (4)
Cd2—O2	2.249 (4)	Cd4—O5^{iii}	2.292 (4)
Cd2—N5	2.248 (4)	Cd4—N7^{iv}	2.319 (4)
Cd2—O3^{i}	2.307 (3)	Cd4—O8	2.337 (4)
Cd2—N6	2.485 (4)	Cd4—O7	2.340 (4)
Cd2—N8	2.567 (4)	Cd4—N13	2.551 (4)
O4^{i}—Cd1—N18^{i}	107.00 (14)	O9^{ii}—Cd3—N12	94.27 (15)
O4^{i}—Cd1—O10^{v}	87.99 (15)	O9^{ii}—Cd3—N17	109.22 (14)
N18^{i}—Cd1—O10^{v}	84.63 (14)	N12—Cd3—N17	144.98 (13)
O4^{i}—Cd1—N3	99.27 (14)	O9^{ii}—Cd3—O1	89.93 (15)
N18^{i}—Cd1—N3	153.12 (13)	N12—Cd3—O1	119.65 (13)
O10^{v}—Cd1—N3	102.16 (15)	N17—Cd3—O1	86.87 (14)
O4^{i}—Cd1—N20^{i}	95.03 (16)	O9^{ii}—Cd3—N15	168.44 (14)
N18^{i}—Cd1—N20^{i}	69.86 (13)	N12—Cd3—N15	92.81 (14)
O10^{v}—Cd1—N20^{i}	154.10 (14)	N17—Cd3—N15	68.94 (13)
N3—Cd1—N20^{i}	102.72 (14)	O1—Cd3—N15	78.63 (14)
O4^{i}—Cd1—N1	161.71 (16)	O9^{ii}—Cd3—N14	95.26 (14)
N18^{i}—Cd1—N1	86.26 (13)	N12—Cd3—N14	68.20 (12)
O10^{v}—Cd1—N1	80.63 (14)	N17—Cd3—N14	83.69 (13)
N3—Cd1—N1	69.57 (13)	O1—Cd3—N14	170.30 (13)
N20^{i}—Cd1—N1	101.47 (15)	N15—Cd3—N14	95.85 (13)
N11—Cd2—O2	81.88 (14)	O6—Cd4—O5^{iii}	110.39 (17)
N11—Cd2—N5	167.65 (15)	O6—Cd4—N7^{iv}	108.65 (17)

O2—Cd2—N5	108.55 (14)	O5^{iii}—Cd4—N7^{iv}	93.07 (17)
N11—Cd2—O3^{i}	98.42 (14)	O6—Cd4—O8	136.16 (15)
O2—Cd2—O3^{i}	95.68 (15)	O5^{iii}—Cd4—O8	86.45 (16)
N5—Cd2—O3^{i}	87.34 (13)	N7^{iv}—Cd4—O8	110.53 (14)
N11—Cd2—N6	102.91 (13)	O6—Cd4—O7	86.30 (16)
O2—Cd2—N6	92.96 (15)	O5^{iii}—Cd4—O7	79.72 (17)
N5—Cd2—N6	70.63 (13)	N7^{iv}—Cd4—O7	164.96 (15)
O3^{i}—Cd2—N6	157.91 (13)	O8—Cd4—O7	56.22 (13)
N11—Cd2—N8	69.63 (13)	O6—Cd4—N13	77.29 (15)
O2—Cd2—N8	151.39 (13)	O5^{iii}—Cd4—N13	170.36 (16)
N5—Cd2—N8	99.49 (14)	N7^{iv}—Cd4—N13	89.76 (14)
O3^{i}—Cd2—N8	91.08 (12)	O8—Cd4—N13	83.93 (13)
N6—Cd2—N8	90.99 (13)	O7—Cd4—N13	95.34 (14)

Symmetry codes: (i) x, -1+y, z; (ii) -x, 1-y, -z; (iii) 1/2-x, 3/2-y, -z; (iv) 1/2+x, 1/2+y, z; (v) -x, -y, -z; (vi) -x, y, 1/2-z.

Complex **4**			
Cd1—O2	2.183 (3)	Cd3—N20	2.489 (3)
Cd1—N5	2.260 (3)	Cd3—N8^{viii}	2.507 (3)
Cd1—N11	2.304 (3)	Cd4—O13	2.241 (3)
Cd1—O10^{vii}	2.322 (3)	Cd4—O7^{ii}	2.253 (3)
Cd1—N13	2.457 (3)	Cd4—O12	2.360 (3)
Cd1—N6	2.523 (3)	Cd4—O3^{iv}	2.398 (3)
Cd2—N17	2.243 (3)	Cd4—N21^{vi}	2.451 (3)
Cd2—O5	2.257 (3)	Cd4—O11	2.455 (3)
Cd2—N4	2.277 (3)	Cd4—O4^{iv}	2.493 (3)
Cd2—O1	2.339 (3)	Cd5—O8^{i}	2.172 (3)
Cd2—N1	2.465 (3)	Cd5—O8^{ii}	2.172 (3)
Cd3—O9	2.170 (3)	Cd5—O11	2.301 (2)
Cd3—N10^{viii}	2.284 (3)	Cd5—O11^{iii}	2.301 (2)
Cd3—N19	2.305 (3)	Cd5—O3^{iv}	2.317 (3)
Cd3—O6	2.329 (3)	Cd5—O3^{v}	2.317 (3)
O2—Cd1—N5	105.46 (12)	N17—Cd2—O5	117.36 (11)
O2—Cd1—N11	101.72 (12)	N17—Cd2—N4	156.21 (11)
N5—Cd1—N11	152.62 (11)	O5—Cd2—N4	86.04 (11)
O2—Cd1—O10^{vii}	86.84 (12)	N17—Cd2—O1	97.53 (11)
N5—Cd1—O10^{vii}	101.99 (11)	O5—Cd2—O1	84.90 (10)
N11—Cd1—O10^{vii}	82.61 (10)	N4—Cd2—O1	88.30 (11)
O2—Cd1—N13	97.50 (12)	N17—Cd2—N1	101.35 (11)
N5—Cd1—N13	103.08 (11)	O5—Cd2—N1	94.72 (11)
N11—Cd1—N13	69.76 (10)	N4—Cd2—N1	70.60 (11)
O10^{vii}—Cd1—N13	152.35 (11)	O1—Cd2—N1	158.86 (11)
O2—Cd1—N6	170.00 (13)	O13—Cd4—O7^{ii}	84.26 (12)
N5—Cd1—N6	68.52 (11)	O13—Cd4—O12	124.47 (11)

N11—Cd1—N6	85.01 (11)	O7^{ii}—Cd4—O12	144.28 (11)
O10^{vii}—Cd1—N6	86.71 (12)	O13—Cd4—O3^{iv}	117.18 (10)
N13—Cd1—N6	91.76 (13)	O7^{ii}—Cd4—O3^{iv}	81.05 (10)
O9—Cd3—N10^{viii}	109.24 (13)	O12—Cd4—O3^{iv}	100.01 (11)
O9—Cd3—N19	101.01 (14)	O13—Cd4—N21^{vi}	83.88 (11)
N10^{viii}—Cd3—N19	146.29 (11)	O7^{ii}—Cd4—N21^{vi}	86.53 (11)
O9—Cd3—O6	85.94 (12)	O12—Cd4—N21^{vi}	77.22 (11)
N10^{viii}—Cd3—O6	114.97 (10)	O3^{iv}—Cd4—N21^{vi}	154.01 (10)
N19—Cd3—O6	81.03 (10)	O13—Cd4—O11	162.28 (10)
O9—Cd3—N20	102.65 (14)	O7^{ii}—Cd4—O11	91.46 (10)
N10^{viii}—Cd3—N20	89.53 (11)	O12—Cd4—O11	54.48 (9)
N19—Cd3—N20	69.22 (10)	O3^{iv}—Cd4—O11	78.89 (9)
O6—Cd3—N20	150.04 (10)	N21^{vi}—Cd4—O11	78.69 (10)
O9—Cd3—N8^{viii}	161.96 (14)	O13—Cd4—O4^{iv}	89.50 (11)
N10^{viii}—Cd3—N8^{viii}	68.73 (10)	O7^{ii}—Cd4—O4^{iv}	123.91 (11)
N19—Cd3—N8^{viii}	86.91 (11)	O12—Cd4—O4^{iv}	81.07 (11)
O6—Cd3—N8^{viii}	79.26 (10)	O3^{iv}—Cd4—O4^{iv}	53.19 (9)
N20—Cd3—N8^{viii}	95.30 (11)	N21^{vi}—Cd4—O4^{iv}	148.08 (10)
O8^{i}—Cd5—O8^{ii}	180.00 (8)	O11—Cd4—O4^{iv}	107.03 (10)
O8^{i}—Cd5—O11	88.08 (11)	O11—Cd5—O3^{iv}	83.80 (10)
O8^{ii}—Cd5—O11	91.92 (11)	O11^{iii}—Cd5—O3^{iv}	96.20 (10)
O8^{i}—Cd5—O11^{iii}	91.92 (11)	O8^{i}—Cd5—O3^{v}	89.10 (11)
O8^{ii}—Cd5—O11^{iii}	88.08 (11)	O8^{ii}—Cd5—O3^{v}	90.90 (11)
O11—Cd5—O11^{iii}	180.00 (18)	O11—Cd5—O3^{v}	96.20 (10)
O8^{i}—Cd5—O3^{iv}	90.90 (11)	O11^{iii}—Cd5—O3^{v}	83.80 (10)
O8^{ii}—Cd5—O3^{iv}	89.10 (11)	O3^{iv}—Cd5—O3^{v}	180.00 (14)

Symmetry codes: (i) 1-x, -y, 1-z; (ii) x, y, -1+z; (iii) 1-x, -y, -z; (iv) 1+x, 1+y, z; (v) -x, -1-y, -z; (vi) 1-x, -1-y, -z; (vii) -1+x, y, z; (viii) 1+x, y, z; (ix) -1+x, -1+y, z; (x) x, y, 1+z.

Complex **5**			
Zn1—O13	2.082 (2)	Zn2—O8^{i}	2.003 (2)
Zn1—O14	2.084 (2)	Zn2—O16	2.047 (2)
Zn1—O1	2.087 (2)	Zn2—N5	2.059 (2)
Zn1—O15	2.090 (2)	Zn2—O17	2.080 (3)
Zn1—N2	2.153 (2)	Zn2—N6	2.224 (2)
Zn1—N3	2.247 (2)	Zn2—O18	2.429 (2)
O13—Zn1—O14	176.20 (8)	O8^{i}—Zn2—O16	89.09 (9)
O13—Zn1—O1	88.17 (8)	O8^{i}—Zn2—N5	173.38 (9)
O14—Zn1—O1	89.16 (9)	O16—Zn2—N5	96.79 (9)
O13—Zn1—O15	95.60 (9)	O8^{i}—Zn2—O17	88.86 (10)
O14—Zn1—O15	87.26 (9)	O16—Zn2—O17	99.16 (10)
O1—Zn1—O15	93.30 (8)	N5—Zn2—O17	93.18 (11)
O13—Zn1—N2	87.53 (9)	O8^{i}—Zn2—N6	97.54 (9)
O14—Zn1—N2	89.80 (9)	O16—Zn2—N6	160.14 (9)

O1—Zn1—N2	90.90 (9)	N5—Zn2—N6	75.91 (9)
O15—Zn1—N2	174.84 (9)	O17—Zn2—N6	99.67 (9)
O13—Zn1—N3	84.48 (9)	O8^{i}—Zn2—O18	92.56 (8)
O14—Zn1—N3	97.57 (9)	O16—Zn2—O18	83.05 (9)
O1—Zn1—N3	166.21 (8)	N5—Zn2—O18	85.17 (9)
O15—Zn1—N3	99.01 (9)	O17—Zn2—O18	177.40 (9)
N2—Zn1—N3	77.16 (9)	N6—Zn2—O18	77.99 (8)

Symmetry codes: (i) 1+x, y, 1+z.